3,5-Dichloronitrobenzene

Other names:	Benzene, 1,3-dichloro-5-nitro- m-Dichloronitrobenzene meta-Dichloronitrobenzene 1,3-Dichloro-5-nitrobenzene 3,5-Dichloro-1-nitrobenzene
Inchi:	InChI=1S/C6H3Cl2NO2/c7-4-1-5(8)3-6(2-4)9(10)11/h1-3H
InchiKey:	RNABGKOKSBUFHW-UHFFFAOYSA-N
Formula:	C6H3Cl2NO2
SMILES:	O=[N+]([O-])c1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	192.00
CAS:	618-62-2

Physical Properties

Property code	Value	Unit	Source
ea	1.55 ± 0.09	eV	NIST Webbook
ea	1.50 ± 0.09	eV	NIST Webbook
gf	104.48	kJ/mol	Joback Method
hf	4.18	kJ/mol	Joback Method
hfus	24.31	kJ/mol	Joback Method
hsub	83.20 ± 1.50	kJ/mol	NIST Webbook
hvap	57.91	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.902		Crippen Method
mcvol	113.540	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	1288.00		NIST Webbook
ripol	1887.00		NIST Webbook
tb	600.02	K	Joback Method
tc	864.46	K	Joback Method
tf	338.00 ± 2.00	K	NIST Webbook
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.83	J/mol×K	600.02	Joback Method
cpg	225.66	J/mol×K	644.09	Joback Method
cpg	232.80	J/mol×K	688.17	Joback Method
cpg	239.30	J/mol×K	732.24	Joback Method
cpg	245.19	J/mol×K	776.31	Joback Method
cpg	250.50	J/mol×K	820.39	Joback Method
cpg	255.28	J/mol×K	864.46	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C618622&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume